The geometric exegesis of the Dirac algorithm

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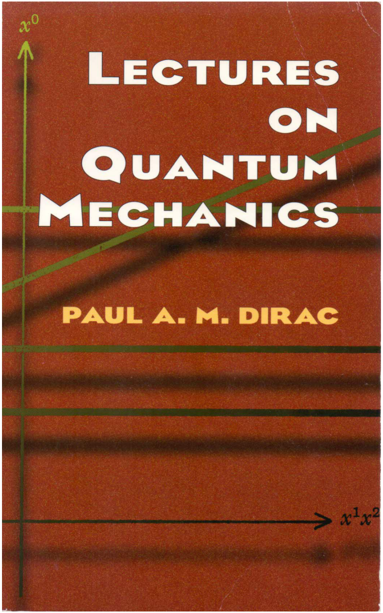
Motivation

back

- Extend the use of Hamiltonian methods to **field theories in bounded regions**. No obstructions in principle but problematic in practice.
- The computation of Poisson brackets when boundaries are present is not trivial. At some point functional-analytic issues become relevant.
- Can we somehow avoid these problems? Yes, but to this end the standard approach must be suitably (subtly?) modified.

A geometric reinterpretation of the usual method helps

exegesis: critical interpretation of a text, particularly a sacred text


x^0
LECTURES
ON
QUANTUM
MECHANICS
PAUL A. M. DIRAC
$x^1 x^2$

The Dirac algorithm in words

- Write the canonical momenta p in terms of q and $\dot{q}$.
- Find the **primary constraints**, i.e. relations $\phi_m(q,p)=0$ between q and p originating in the "impossibility to solve for all the velocities" in terms of positions and momenta.
- Find a Hamiltonian H and build the **total Hamiltonian** $H_T = H + \sum u_m\phi_m$ in which the **primary constraints** are introduced together with some multipliers $u_m(t)$.
- The u_m must be fixed by enforcing the **consistency of the time evolution of the system.** This consistency requires, for instance, that the primary constraints be **preserved in time**:

$$\boxed{\{\phi_m, H\} + u_n\{\phi_m, \phi_n\} \approx 0}$$

  The weak equality symbol $\approx$ means that the previous identity must hold when the primary constraints are enforced.

The Dirac algorithm in words (continued)

- **Several possibilities:**

  1. The consistency conditions may be **impossible to fulfill**. This means that our starting point (the Lagrangian) makes no sense.
  2. The consistency conditions may be trivial, i.e. identically satisfied once the primary constraints are enforced.
  3. The u_m **may not appear** in the consistency conditions. In this case we have **secondary constraints**.
  4. The consistency conditions can be solved for the u_m.

- If we find secondary constraints their "**stability** under time evolution" **must be enforced**, exactly as we did for the primary constraints. However **we do not have to modify the total Hamiltonian** (i.e. we do not have to include them in a new, "more total" Hamiltonian).

The Dirac algorithm in words (continued)

- Let us look with some care at the equations

$$\boxed{\{\phi_j, H\} + u_n\{\phi_j, \phi_n\} \approx 0}$$

- These are **linear**, **inhomogeneous** equations for the unknowns u_n. As such, the inhomogeneous term will be subject, generically, to conditions necessary to guarantee solvability.
- **These are the secondary constraints**. Their number is determined by the **rank of the matrix** $\{\phi_j, \phi_n\}$ (beware of *bifurcation*!).
- Once solvability is guaranteed we can find the u_n (as functions of the generalized coordinates and momenta) and, maybe, arbitrary parameters.

$$\boxed{u_m = U_m(q, p) + v_a(t) V_{am}(q, p)},$$

where $V_{an}\{\phi_j, \phi_n\} = 0$ and the $v_a(t)$ are arbitrary functions of time.

The Hamiltonian $\hat{\mathrm{H}} = \mathrm{H} + (U_m(q,p) + v_a(t)V_{am}(q,p))\phi_m$ defines **consistent dynamics** equivalent to the one given by the singular Lagrangian used to define our system **for initial data for** (q,p) **satisfying all the constraints** (primary and secondary).

Comments on the Dirac algorithm

- Its logic is difficult to follow at times. For instance, sentences such as

  The Poisson bracket $[g, u_m]$ *is not defined, but it is multiplied by something that vanishes,* ϕ_m*. So the first term of (1-18) vanishes.* (P.A.M. Dirac, LQM)

  sound strange.
- It is not so straightforward to extended it to field theories.
- This notwithstanding, **the algorithm works well if followed to the letter!** (and if the results are correctly interpreted).

Scalar field with Dirichlet boundary conditions back

$$S[\varphi,\psi_0,\psi_1]=\int_{t_1}^{t_2}\mathrm{d}t\left[\frac{1}{2}\int_0^1\mathrm{d}x(\dot{\varphi}^2-\varphi'^2)-\psi_0\big(\varphi(0)-\varphi_0\big)+\psi_1\big(\varphi(1)-\varphi_1\big)\right]$$

- The configuration variables are $\varphi(x)$, ψ_0 and ψ_1.
- ψ_0 and ψ_1 are Lagrange multipliers introduced to enforce the boundary conditions $\varphi(0)=\varphi_0$ and $\varphi(1)=\varphi_1$.
- $\varphi_0\,,\varphi_1\in\mathbb{R}$, (boundary values of φ).
- $\varphi\in C^2(0,1)\cap C^1[0,1]$ (smooth enough).

Do we get the right field equations?

We should better check...

Scalar field with Dirichlet boundary conditions back

Field equations: variations of the action

$$
\begin{aligned}
\delta S \;=\;& \int_{t_1}^{t_2} \mathrm{d}t \left(\int_0^1 \mathrm{d}x(-\ddot{\varphi}(x) + \varphi''(x))\delta\varphi(x) - \varphi'(x)\delta\varphi(x)\Big|_0^1 \right) \\
&- \int_{t_1}^{t_2} \mathrm{d}t(\varphi(0) - \varphi_0)\delta\psi_0 + \int_{t_1}^{t_2} \mathrm{d}t(\varphi(1) - \varphi_1)\delta\psi_1 \\
&- \int_{t_1}^{t_2} \mathrm{d}t\psi_0\delta\varphi(0) + \int_{t_1}^{t_2} \mathrm{d}t\psi_1\delta\varphi(1)
\end{aligned}
$$

$$
\begin{aligned}
&\ddot{\varphi}(x) - \varphi''(x) = 0\,, \quad x \in (0,1) \\
&\varphi(0) = \varphi_0 \\
&\varphi(1) = \varphi_1 \qquad \checkmark \\
&\psi_1 - \varphi'(1) = 0 \\
&\psi_0 - \varphi'(0) = 0
\end{aligned}
$$

Scalar field with Dirichlet boundary conditions back

- **Canonical momenta**:

$$\pi(x) := \frac{\delta\mathcal{L}}{\delta\dot{\varphi}(x)} = \dot{\varphi}(x)\,,\, p_0 := \frac{\partial\mathcal{L}}{\partial\dot{\psi}_0} = 0\,,\, p_1 := \frac{\partial\mathcal{L}}{\partial\dot{\psi}_1} = 0$$

- **Primary constraints** $p_0 = 0$ and $p_1 = 0$.
- Non-zero **Poisson brackets**

$$\{\varphi(x), \pi(y)\} = \delta(x, y)\,,\, \{\psi_0, p_0\} = 1\,,\, \{\psi_1, p_1\} = 1$$

- **Total hamiltonian**

$$H_T = \psi_0\big(\varphi(0) - \varphi_0\big) - \psi_1\big(\varphi(1) - \varphi_1\big) + u_0 p_0 + u_1 p_1 + \frac{1}{2}\int_0^1 \mathrm{d}x\big(\pi^2 + \varphi'^2\big)\,.$$

- Here u_0 and u_1 are the Lagrange multipliers that enforce the primary constraints in the Dirac algorithm.

Before going further just a short question...

Scalar field with Dirichlet boundary conditions back

What is the value of $\{\varphi(0), \pi(0)\}$?, Is it 1?, Is it $\delta(0,0)$?

This is not an academic question

Secondary constraints (at $x = 0$, analogously at $x = 1$)

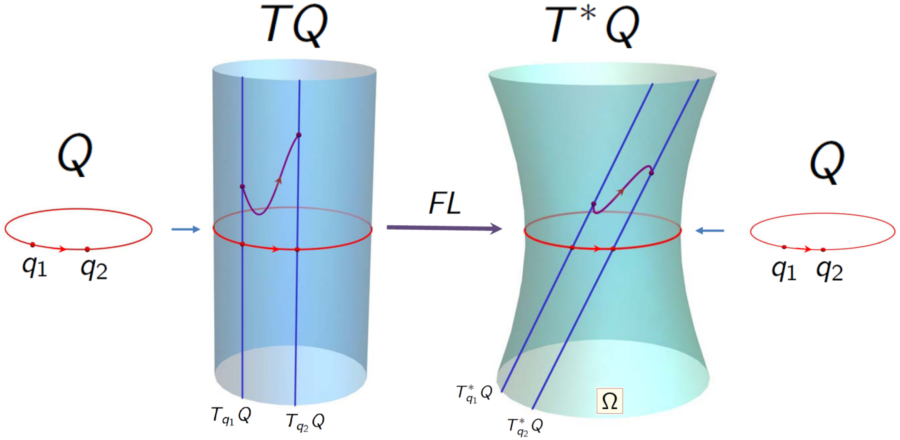
$$\{H_T, p_0\} = \varphi(0) - \varphi_0 = 0 \quad \text{(OK)}$$

$$\{H_T, \varphi(0) - \varphi_0\} = \int_0^1 \mathrm{d}x\pi(x) \underbrace{\{\pi(x), \varphi(0)\}}_{-\delta(x,0)} = -\pi(0) = 0 \quad \text{(uhm...)}$$

$$\begin{aligned}\{H_T, \pi(0)\} &= \{\varphi(0), \pi(0)\}\psi_0 + \int_0^1 \mathrm{d}x\varphi'(x)\{\varphi'(x), \pi(0)\} \\ &= \{\varphi(0), \pi(0)\}\psi_0 + \varphi'(x)\{\varphi(x), \pi(0)\}\Big|_0^1 \\ &\quad - \int_0^1 \mathrm{d}x\varphi''(x)\{\varphi(x), \pi(0)\} \quad \text{(???)}\end{aligned}$$

The algorithm **crashes**. One has to be careful...

Geometric interpretation of the Dirac algorithm back



The geometric exegesis of the Dirac algorithm, preliminaries.

- The goal is to find a Hamiltonian H defined **on the whole phase space** such that the integral curves of the Hamiltonian vector field X_H describe the dynamics of the system for **allowed initial data**. This is important to implement the quantization programme *à la Dirac*.
- The dynamics must take place **on the primary constraint** submanifold of the phase space given by $FL(TQ)$ (the image of the fiber derivative defining the momenta).
- The Hamiltonian vector field, when restricted to the submanifold where the dynamics takes place, **must be tangent to it** (otherwise the integral curves would fail to remain there!)

The gist of Dirac's algorithm is this tangency condition

The geometric exegesis of the Dirac algorithm (continued).

- The starting point is the identification of the **primary constraints** ϕ_n. These are found by computing the **fiber derivative** (definition of momenta)
$$\boxed{FL : TQ \to T^*Q}$$
- From the energy E we get the **Hamiltonian** from $H \circ FL = E$ (a real function in T^*Q which is uniquely defined only on the **primary constraint submanifold** $\mathcal{M}_0 := FL(TQ)$, given by **constraints** $\phi_n = 0$).
- Find the vector fields X satisfying
$$\boxed{\imath_X \Omega - \mathrm{d}H - u_n \mathrm{d}\phi_n = 0}$$
and require also
$$\boxed{\phi_n(q,p) = 0}\,.$$

Singular Hamiltonian systems: the Dirac algorithm

back

The geometric exegesis of the Dirac algorithm, (continued).

- In order to have consistent dynamics we must require X to be **tangent** to the primary constraint submanifold $\mathcal{M}_0$.

$$\boxed{\imath_X \mathrm{d}\phi_n \big| \mathcal{M}_0 = 0}$$

  $\imath_X \mathrm{d}\phi_n$ just gives, at each point, the **directional derivative** of ϕ_n along X. Notice that it can be computed *without using the symplectic form.*
- Three things may happen at this point:
  1. The tangency condition is **identically satisfied**.
  2. The tangency condition is only satisfied **on a proper submanifold** of the primary constraint submanifold.
  3. The tangency condition **fixes some** of the arbitrary u_n.

The geometric exegesis of the Dirac algorithm, (continued).

- In the **first case** we are done.
- In the **second case** the conditions defining the submanifold are **secondary constraints**. The Hamiltonian vector field X will be tangent to the primary constraint manifold but **may fail to be tangent to the new submanifold**. If this is the case we must persevere with tangency.
- In the **third case** the specific values of u_n, when introduced in X will give us a Hamiltonian vector field defining the right evolution.

The dynamics that we obtain by projecting the integral curves of the Hamiltonian vector fields onto Q is the same as the Lagrangian dynamics. We also obtain the additional conditions that the initial data (on the generalized positions and momenta) must satisfy.

Scalar field with Dirichlet boundary conditions back

(Homogeneous conditions $\varphi(0) = \varphi(1) = 0$)

Lagrangian

$$L(\mathrm{v}) = \frac{1}{2}\int_0^1 \left(v_\varphi^2 - \varphi'^2 + 2\,(\psi\varphi)'\right)$$

Fiber derivative

$$\langle FL(\mathrm{v})|\mathrm{w}\rangle \;=\; \int_0^1 v_\varphi w_\varphi, \quad \longrightarrow \quad \begin{array}{l} \mathbf{p}_\varphi(\cdot) := \displaystyle\int_0^1 v_\varphi \,\cdot\,, \\[2ex] \mathbf{p}_\psi(\cdot) := 0\,. \end{array}$$

Hamiltonian (extension to the full phase space)

$$H = \frac{1}{2}\int_0^1 \left(p_\varphi^2 + \varphi'^2 - 2\,(\psi\varphi)'\right)\,,$$

Scalar field with Dirichlet boundary conditions back

Vector fields

$$Y \in T_{(\varphi,\psi;p_\varphi,p_\psi)} T^*\mathcal{Q} \to Y = \big((\varphi,\psi;p_\varphi,p_\psi),(Y_\varphi, Y_\psi, \boldsymbol{Y}_{\mathbf{p}_\varphi}(\cdot), \boldsymbol{Y}_{\mathbf{p}_\psi}(\cdot))\big)\,.$$

$\boldsymbol{Y}_{\mathbf{p}_\varphi}(\cdot)$, $\boldsymbol{Y}_{\mathbf{p}_\psi}(\cdot)$ can be represented by real functions $Y_{\mathbf{p}_\varphi}$, $Y_{\mathbf{p}_\psi}$ such that over functions $f, g \in \mathcal{Q}$

$$\boldsymbol{Y}_{\mathbf{p}_\varphi}(f) := \int_0^1 Y_{\mathbf{p}_\varphi} f\,, \quad \boldsymbol{Y}_{\mathbf{p}_\psi}(g) := \int_0^1 Y_{\mathbf{p}_\psi} g\,.$$

Differential of H acting on a vector field Y

$$\mathrm{d}H(Y) = \int_0^1 \left(Y_{p_\varphi} p_\varphi - \varphi'' Y_\varphi\right) - \left[\left(\psi - \varphi'\right) Y_\varphi + \varphi Y_\psi\right](1) + \left[\left(\psi - \varphi'\right) Y_\varphi + \varphi Y_\psi\right](0)\,.$$

Canonical symplectic form in $T^*\mathcal{Q}$, acting on a pair of vector fields X, Y

$$\Omega(X,Y) = \int_0^1 \left(Y_{p_\varphi} X_\varphi - X_{p_\varphi} Y_\varphi + Y_{p_\psi} X_\psi - X_{p_\psi} Y_\psi\right)\,.$$

Scalar field with Dirichlet boundary conditions back

We solve for X in the equation (for all Y)

$$\Omega(X,Y) = \mathbf{d}H(Y) + \langle \mathbf{u} | \mathbf{d}p_\psi \rangle (Y) = \mathbf{d}H(Y) + \int_0^1 u Y_{p_\psi}$$

By considering first fields Y vanishing at 0 and 1 we get the Hamiltonian vector field X in the interval $[0,1]$

$$X_\varphi = p_\varphi \,, \qquad X_\psi = u \,,$$
$$X_{p_\varphi} = \varphi'' \,, \qquad X_{p_\psi} = 0 \,.$$

Once we know X, we can allow Y to be **arbitrary on the boundary**. This gives us, then, the following **secondary constraints**

$$\varphi(0) = 0 \qquad \varphi(1) = 0 \,, \tag{1}$$
$$\psi(0) - \varphi'(0) = 0 \qquad \psi(1) - \varphi'(1) = 0 \,, \tag{2}$$

which include both the **Dirichlet boundary conditions** and the **values of ψ at the boundary**. This is the result given by the Euler-Lagrange equations.

Scalar field with Dirichlet boundary conditions back

We must check now the tangency of the Hamiltonian field, to the submanifold in $T^*\mathcal{Q}$ defined by the constraints $p_\psi = 0$ and the boundary conditions

Tangency of the Hamiltonian vector field

$$0 = \imath_X \mathbf{d} p_\psi = X_{p_\psi} \,,$$
$$0 = \imath_X \mathbf{d}\left(\varphi(j)\right) = X_\varphi(j) = p_\varphi(j)\,, \quad j \in \{0,1\}$$
$$0 = \imath_X \mathbf{d}\left(\psi(j) - \varphi'(j)\right) = X_\psi(j) - X'_\varphi(j) = u(j) - p'_\varphi(j) \quad j \in \{0,1\}\,.$$

- The first gives nothing new.
- The next pair of conditions are new secondary constraints at 0 and 1.
- The last pair fixes the Dirac multiplier at the boundary $u(0) = p'_\varphi(0)$, $u(1) = p'_\varphi(1)$.

Scalar field with Dirichlet boundary conditions back

We must demand now that the vector field X be tangent to the new submanifold defined by the secondary constraints just obtained. These **new tangency conditions** give

$$0 = \imath_X \mathbf{d}\,(p_\varphi(j)) = X_{p_\varphi}(j) = D^2\varphi(j)\,, \quad j \in \{0,1\}$$

where D^n denotes the n-th order spatial derivative.

As we see, there are **more secondary constraints** and **additional tangency requirements**. Iterating this process, we find an **infinite number of boundary constraints** of the form ($n \in \mathbb{N}$)

$$\begin{aligned} D^{2n}\varphi(0) &= 0\,, & D^{2n}p_\varphi(0) &= 0\,,\\ D^{2n}\varphi(1) &= 0\,, & D^{2n}p_\varphi(1) &= 0\,. \end{aligned}$$

Scalar field (final result)

back

Hamiltonian vector field

$$X_\varphi = p_\varphi\,, \qquad X_\psi = u\,,$$
$$X_{p_\varphi} = \varphi''\,, \qquad X_{p_\psi} = 0\,.$$

Primary constraints

$$\boxed{\mathbf{p}_\psi(\cdot) := 0}$$

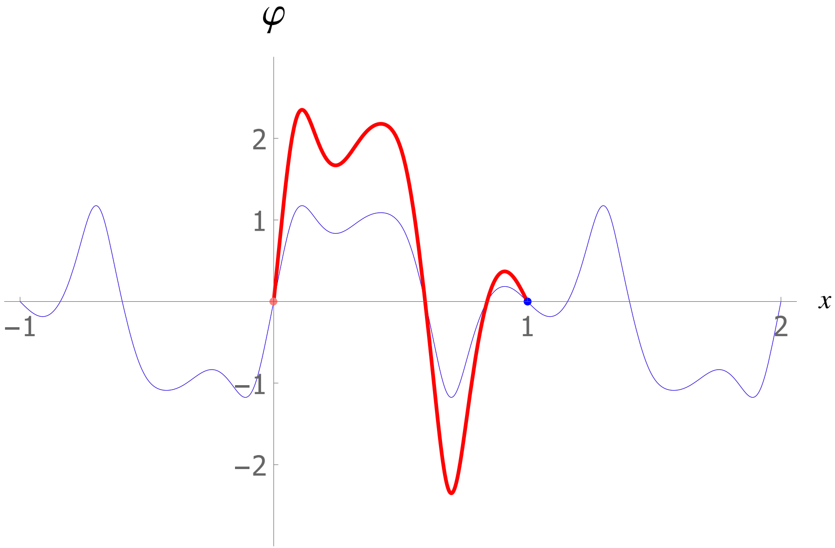
Secondary constraints

$$\varphi(0) = 0\,, \quad \varphi(1) = 0$$
$$\psi(0) - \varphi'(0) = 0\,, \quad \psi(1) - \varphi'(1) = 0$$
$$p_\varphi(0) = 0\,, \quad p_\varphi(1) = 0$$
$$D^{2n}\varphi(0) = 0\,, \quad D^{2n}\varphi(1) = 0 \quad n \in \mathbb{N}$$
$$D^{2n}p_\varphi(0) = 0\,, \quad D^{2n}p_\varphi(1) = 0 \quad n \in \mathbb{N}$$

The Lagrange multiplier u is **arbitrary** in $(0,1)$ but $u(0) = u(1) = 0$

Scalar field with Dirichlet boundary conditions back

Meaning of the boundary constraints $D^{2n}\varphi(j) = 0\,, D^{2n}p_\varphi(j) = 0\,, j = 0\,,1$



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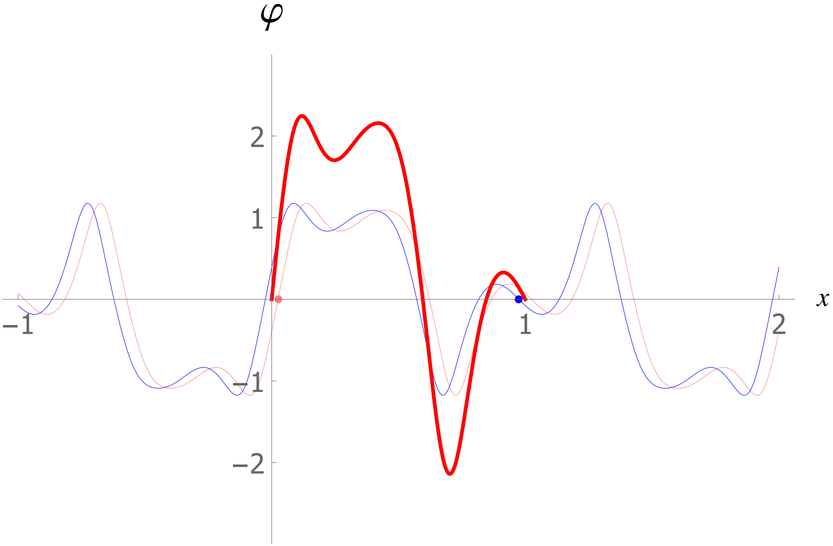

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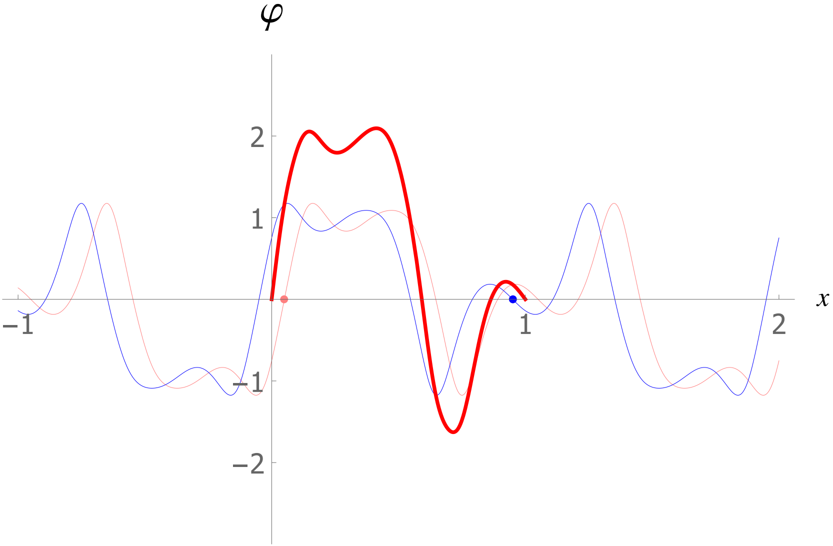

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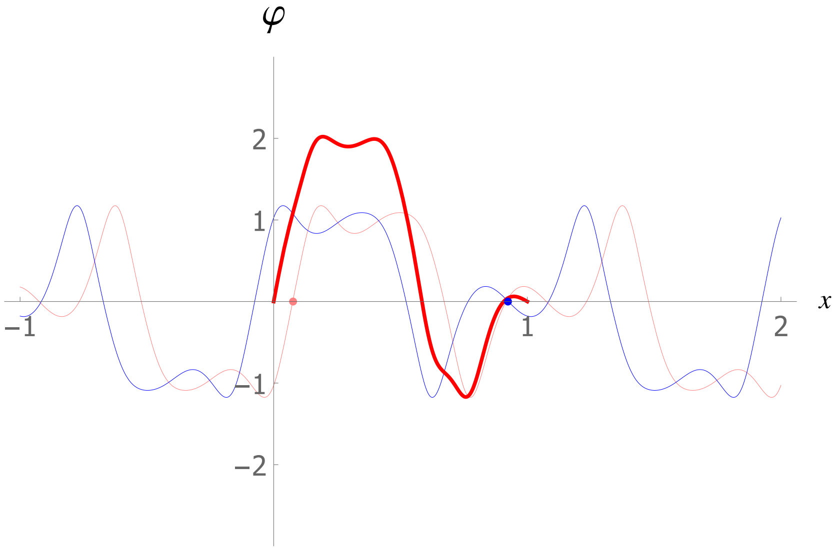

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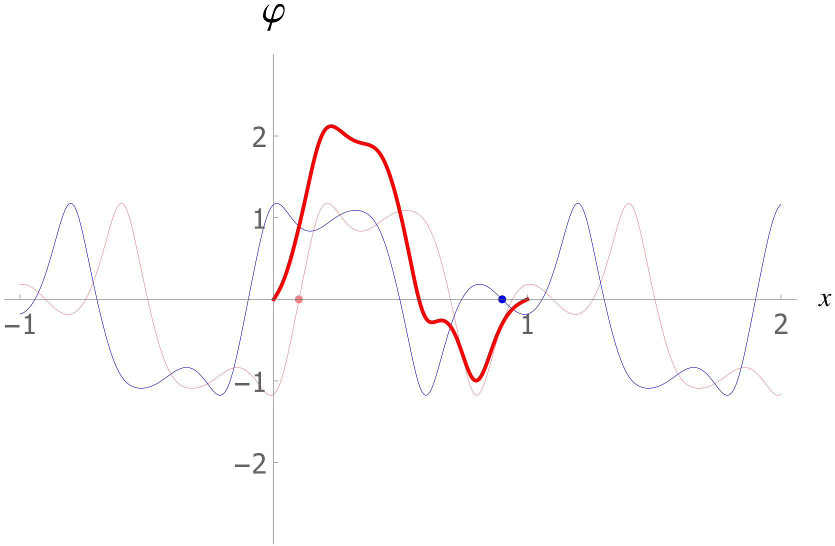

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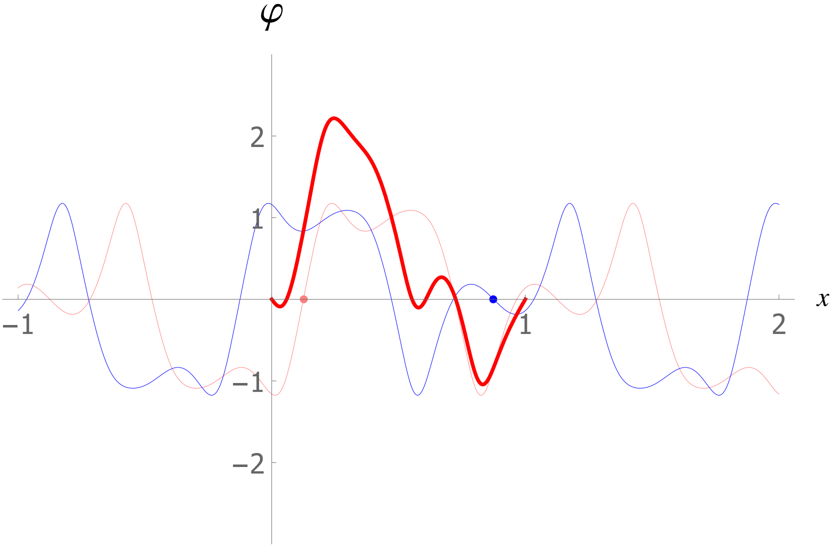

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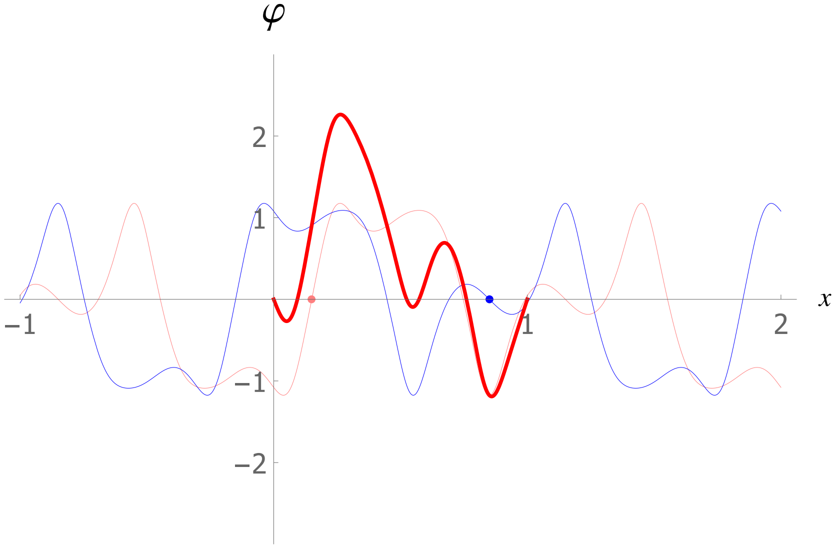

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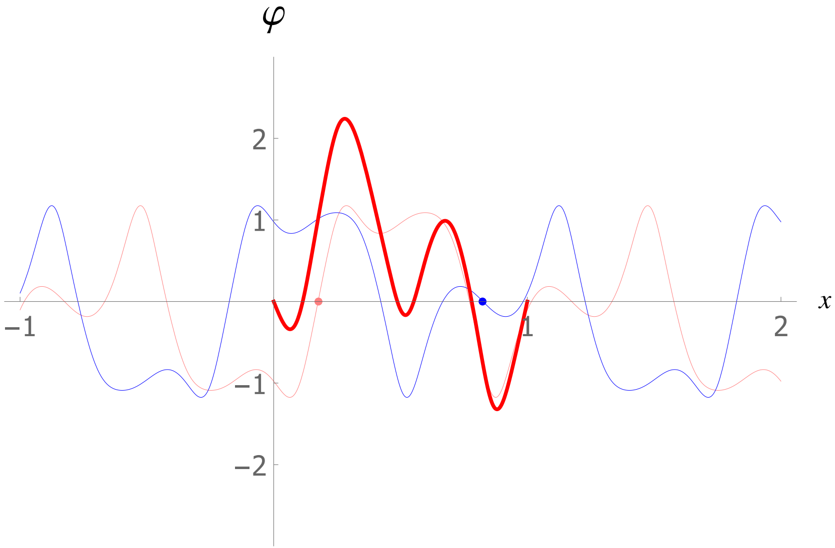

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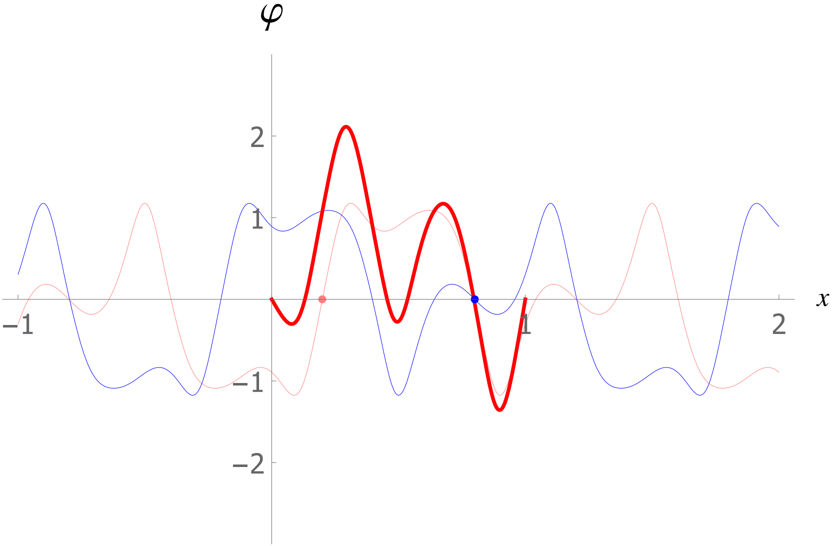

Conclusions

back

The geometric approach to the Dirac algorithm

- The steps of the Dirac algorithm can be conveniently interpreted in **geometric terms**.
- The stability of the constraints is the **tangency condition** of the constraint submanifold to the Hamiltonian vector field.
- Actual computations can be performed in a way that avoids the use of formal Poisson brackets. This is sometimes useful, for instance, for **field theories in bounded regions**.
- In practice the computations are rather clean and quick.
- A similar approach—the so called Gotay-Nester-Hinds (GNH) method—does a similar thing on the primary constraint submanifold.

Conclusions

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Happy birthday, Jurek!!